Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

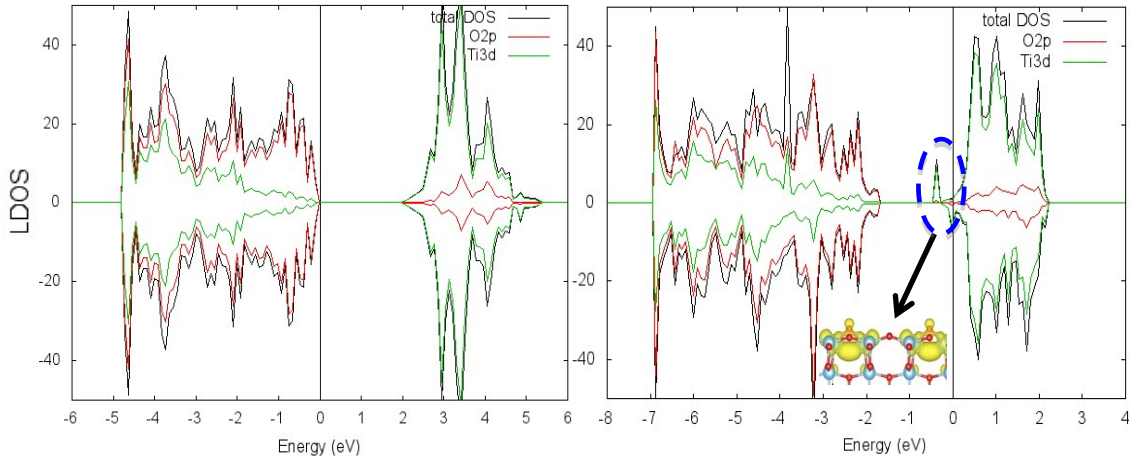

Fig. S1. Local Density of States (LDOS) of **(a)** pristine and, **(b)** defective *anatase* TiO_2 (001) with surface O_{vac} calculated at DFT-D2. Negative and positive values of y-axis are minority and majority spin, respectively. Fermi level is set to 0 eV. (Isosurface = 0.02 e/Å^3)

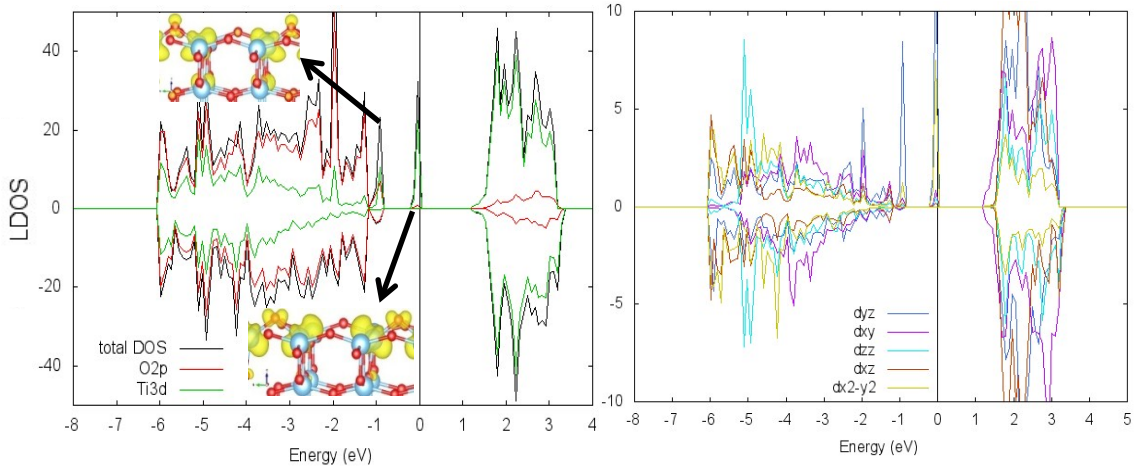

Fig. S2. LDOS of reduced *anatase* TiO_2 (001) surface calculated at DFT-D2+U_d (U_d = 4 eV). (Isosurface = 0.02 e/Å^3)

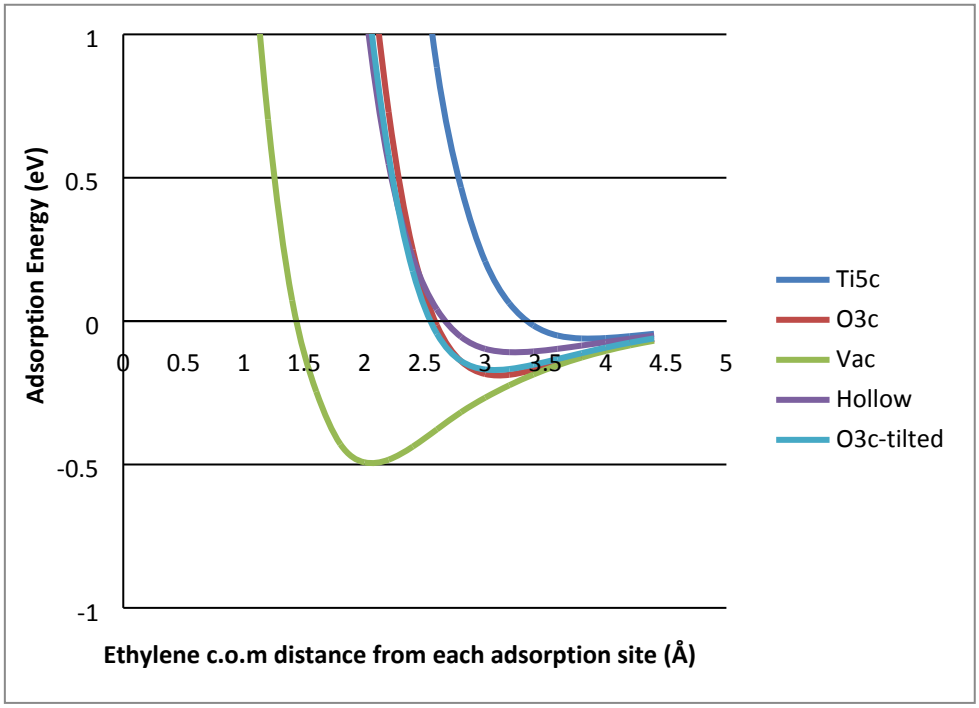

Fig. S3. Potential Energy Curve (PEC) of ethylene adsorption on five adsorption sites considered in this work. The calculations were done using DFT-D2+U_d (U_d=3eV).

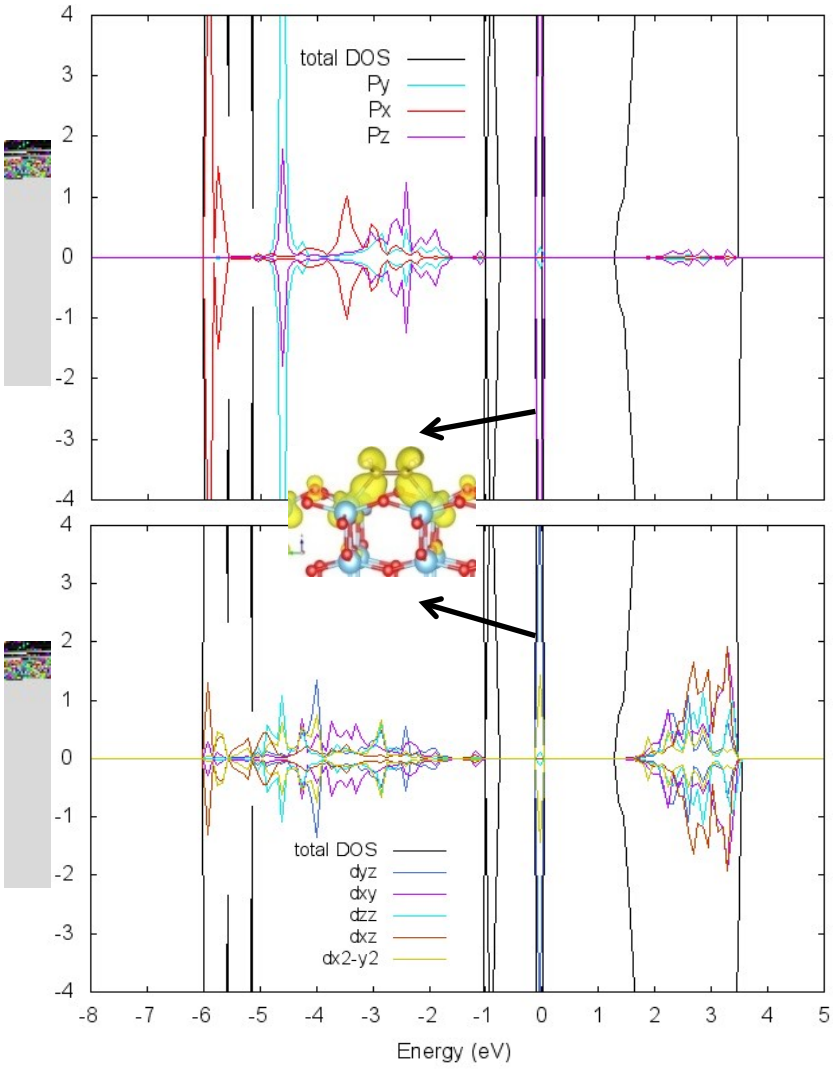

Fig. S4. LDOS of ethylene adsorbed on O_{vac}-site calculated at DFT-D2+U_d (U_d = 4 eV) and the corresponding partial charge density of the newly formed mid-gap state. **(a)** orbital-resolved LDOS of ethylene's two C-atom projected onto their 2*p*-state plotted together with total DOS, **(b)** orbital-resolved LDOS of the two Ti-atom near the O_{vac} projected onto their

Site	ΔE_{ads} (eV)	d C=C (Å)	d C-H (Å)	d C-Ti (Å)
Ti_{5c}	-- **[-0.10]**	-- **[1.34]**	-- **[1.09]**	-- **[3.25]**
O_{3c}	-0.01 **[-0.20]**	1.34 **[1.34]**	1.09 **[1.09]**	3.85 **[3.47]**
O_{2c}	-1.04 **[-1.50]**	1.49 **[1.50]**	1.11 **[1.11]**	2.11 **[2.11]**
Hol	-0.02 **[-0.41]**	1.33 **[1.33]**	1.09 **[1.09]**	3.73 **[3.48]**
O_{3c} tilted	-0.06 **[-0.30]**	1.34 **[1.34]**	1.09 **[1.09]**	3.52 **[3.31]**

Table S1. Calculated adsorption energies and selected geometrical parameters of adsorbed ethylene on different configurations. Values outside the bracket were calculated at DFT/GGA and those in the brackets were calculated at DFT/GGA-D2 level.